Ethylbenzene

Lityibotizotio							
100-41-4 DTXSID3020596							

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.27

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

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Ethylbenzene Measured: 3.15 Predicted: 3.27 Image not found

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Measured: 3.18 Predicted: 2.98

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3-fluoropropylbenzene Measured: 2.95 Predicted: 3.43

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Propylbenzene Measured: 3.69 Predicted: 3.68 Image not found

alpha-Methylstyrene Measured: 3.48 Predicted: 3.23